MATH858T Maria Cameron

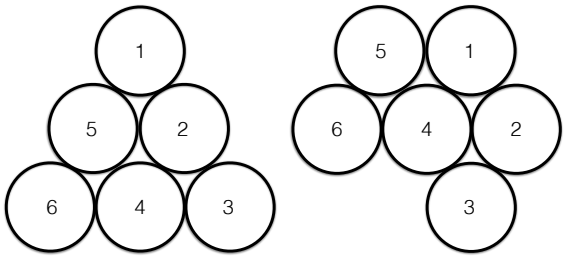
Homework 10. Due May 6.

Consider 6 atoms in 2D interacting according to the Lennard-Jones pair potential. The potential energy of this system is given by

$$V = 4\sum_{i=1}^{5}\sum_{j=i+1}^{6}(r_{ij}^{-12} - r_{ij}^{-6}), \quad r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}.$$

The goal of this problem is to practice the string method for finding transition paths and the shrinking dimer method for finding saddle points in gradient SDEs. The endpoints for the string method, functions for computing the gradient and the potential energy, and a function for visualizing configurations and transition paths are provided in `LJ6in2Dsetup.m`.

1. **(6 points)** Use the string method to find the Minimum Energy Path connecting the following two configurations:



   Plot the energy along the found Minimum Energy Path.

2. **(6 points)** Use the shrinking dimer method to find the saddle point(s) encountered by the found Minimum Energy Path. Make your code display the found saddle(s) and the potential energy at it (them) and indicate the norm of the gradient of the potential at the saddle(s) (it should be small, less than your tolerance, but it will not be exactly zero).